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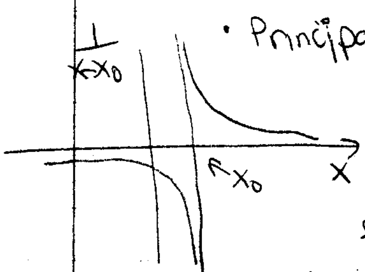
834 Lecture 7

Lecture plan: (many small, related topics)

- Comments on the midterm (63)
- Recap Legendre function → polynomials (60), (61)
- Mathematica and differential equations (64), (65)
- Analytic continuation and gamma function (48), (66), (67)
- Harmonic functions
- Asymptotic methods
- Setting up PS#4 problems
- Solving S eqn for bound states (Numerov method)
- Fourier series introduction.

Before class:

- Start up Mathematica and bring up PS#3 notebook
- Principal value recap



$$P\int_{-\infty}^{\infty}\frac{1}{x-x_0}dx = \left[\int_{-\infty}^{x_0-\varepsilon} + \int_{x_0+\varepsilon}^{\infty}\right]\frac{1}{x-x_0}dx = 0$$ because the areas cancel as long as we integrate symmetrically about $x=x_0$. If we have $\frac{f(x)}{x-x_0}$, the areas still cancel, because $f(x_0\pm\varepsilon) \doteq f(x_0)$ and we can pull $f(x)$ outside the integral.

On board: · Legendre Function recap

$$(1-x^2)y'' - 2xy' + \alpha(\alpha+1)y = 0$$

consider each in general

$$y = \sum_{n=0}^{\infty} a_n x^{n+k} \Rightarrow \quad n=0,\ x^{k-2}:\ k(k-1)a_0 = 0 \Rightarrow k=0 \text{ or } k=1$$

$n=1,\ x^{k-1}:\ (k+1)\cdot k\, a_1 = 0 \Rightarrow$ possible constraints on a_1; not additional k's.

$$k=0 \quad a_{j+2} = \frac{j(j+1)-\alpha(\alpha+1)}{(j+2)(j+1)}a_j \quad \Big| \quad k=1:\ a_{j+2} = \frac{(j+1)(j+2)-\alpha(\alpha+1)}{(j+3)(j+2)}a_j$$

$\alpha = l$ integer (angular momentum) $\Rightarrow$ Legendre polynomials

Here: unnormalized polynomials $y_0(x)=1$, $y_1(x)=x$, $y_2(x)=1-3x^2$, ...

Later: $P_0(x)=1$, $P_1(x)=x$, $P_2(x)=\frac{1}{2}(3x^2-1)$, ... $\Rightarrow \int_{-1}^{1}P_l(x)P_{l'}(x)dx = \frac{2}{2l+1}\delta_{ll'}$ on $[-1,1]$

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Comments on the upcoming midterm

- Wednesday during class. Design is for one-hour exam, but you have the full 1 hour 48 minute period to do it.

- Two parts: basic problems, synthetic problems
  - basics: testing for core competencies
    - what everyone needs to know to pass
    - e.g., δ_{ij} and ε_{ijk} manipulations; applying formulas on Jackson covers; knowing different types of singularities; complex manipulations (like taking n^{th} roots); applying Frobenius
    - "Spot the error!"

  what does 'analytic' entail?

  Aside: What functions have branch points? $f(z)=(z-z_0)^{\alpha}$ ← $\alpha \neq$ integer, $\ln(z-z_0)$
  - Non-analytic at $z_0 \Rightarrow$ Taylor series doesn't exist. Seen here by derivatives (eventually) blowing up at z_0 eg.

    $f(z)=(z-z_0)^{3/2}$, $f'(z)=3/2(z-z_0)^{1/2}$ $f''(z)=\frac{3}{2}\cdot\frac{1}{2}(z-z_0)^{-1/2} \Rightarrow f''(z_0)=\infty$

  - synthetic: putting ideas/techniques together; applying to new situations

- Based on topics seen in homework problems
  - Items, setting up problems, applying tools like δ_{ij}, ε_{ijk}, definitions and notation

- You will be given Jackson covers; any needed integrals like $\int_0^{\infty} e^{-r^2} dr$
- You will not be given (must know these!)

  $e^{iz} = \cos z + i \sin z = 1 + z + \frac{z^2}{2!} + \ldots$ $\qquad (1+z)^{\alpha} = 1 + \alpha z + \ldots \quad |z|<1$

  $\varepsilon_{abc}\varepsilon_{ade} = \delta_{bd}\delta_{ce} - \delta_{be}\delta_{cd}$ "All numbers in ε_{abc} must be different. If first indices are the same, then either the next two and the last two are the same; or the 2nd and 3rd of each are the same, with a minus sign."

  - CR relations, shouldn't have to memorize.

- How to prepare:
  - Go over PS#1–4 and make sure you can set up every problem without looking at solutions
  - Check solutions and lecture notes for emphasis points. Remember the picky points taken off on homework and emphasized in class

Differential Equations in *Mathematica*: PS#3 examples

PS#3 Problem 4

note need y''[x], not just y''

Try to find a general solution to PS #3, Problem 4

```
In[1]:= DSolve[x y''[x] + (1 - x) y'[x] + α y[x] == 0, y, x]

Out[1]= {{y → Function[{x}, C[1] HypergeometricU[-α, 1, x] + C[2] LaguerreL[α, x]]}}
```

Perhaps not so helpful because these are general functions (look them up in the Documentation Center). To see the polynomial solutions we can try a specific value, such as α=2:

```
In[2]:= DSolve[x y''[x] + (1 - x) y'[x] + 2 y[x] == 0, y, x]

Out[2]= {{y → Function[{x}, (2 + (-4 + x) x) C[1] +
          1/4 C[2] (3 e^x - e^x x + 2 ExpIntegralEi[x] - 4 x ExpIntegralEi[x] + x^2 ExpIntegralEi[x])]}}
```

Ok, that gives our polynomial and another cryptic function: ExpIntegralEI (look it up!).

Define a function that let's us easily change the integer:

```
In[3]:= prob4[n_] := DSolve[x y''[x] + (1 - x) y'[x] + n y[x] == 0, y, x]
```

Test it

```
In[4]:= prob4[0]

Out[4]= {{y → Function[{x}, C[2] + C[1] ExpIntegralEi[x]]}}
```

Good, but awkward. Let's strip out the excess baggage:

```
In[5]:= prob4full[n_] := (y[x] /. DSolve[x y''[x] + (1 - x) y'[x] + n y[x] == 0, y, x])[[1]]
```

The [[1]] gets rid of the final {}'s. It refers to a part of the equation. Look up Part in the help for examples of this very useful capability.

```
In[6]:= prob4full[0]

Out[6]= C[2] + C[1] ExpIntegralEi[x]

In[7]:= ? ExpIntegralEi
```

ExpIntegralEi[z] gives the exponential integral function Ei(z). >>

Expand to see the logarithm

```
In[8]:= Simplify[Series[ExpIntegralEi[x], {x, 0, 4}], Assumptions → {x > 0}]
```

Out[8]= $(\text{EulerGamma} + \text{Log}[x]) + x + \frac{x^2}{4} + \frac{x^3}{18} + \frac{x^4}{96} + O[x]^5$

```
In[9]:= EulerGamma // N

Out[9]= 0.577216
```

The solution with ln x is discussed in the Arfken and Lea texts.

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In[10]:= **prob4full[1]**

Out[10]= $(-1+x)\,C[1]+C[2]\,(-e^x-\text{ExpIntegralEi}[x]+x\,\text{ExpIntegralEi}[x])$

In[11]:= **prob4full[2]**

Out[11]= $(2+(-4+x)\,x)\,C[1]+\frac{1}{4}C[2]\left(3e^x-e^x x+2\,\text{ExpIntegralEi}[x]-4x\,\text{ExpIntegralEi}[x]+x^2\,\text{ExpIntegralEi}[x]\right)$

In[12]:= **prob4full[3]**

Out[12]= $(-6+(-6+x)\,(-3+x)\,x)\,C[1]+\frac{1}{36}C[2]\left(-11e^x+8e^x x-e^x x^2-6\,\text{ExpIntegralEi}[x]+18x\,\text{ExpIntegralEi}[x]-9x^2\,\text{ExpIntegralEi}[x]+x^3\,\text{ExpIntegralEi}[x]\right)$

In[13]:= **prob4full[4]**

Out[13]= $(24+(-4+x)\,x\,(24+(-12+x)\,x))\,C[1]+\frac{1}{576}C[2]\left(50e^x-58e^x x+15e^x x^2-e^x x^3+24\,\text{ExpIntegralEi}[x]-96x\,\text{ExpIntegralEi}[x]+72x^2\,\text{ExpIntegralEi}[x]-16x^3\,\text{ExpIntegralEi}[x]+x^4\,\text{ExpIntegralEi}[x]\right)$

What about non-integers?

In[14]:= **prob4full[1 / 2]**

Out[14]= $C[1]\,\text{HypergeometricU}\left[-\frac{1}{2},1,x\right]+C[2]\,\text{LaguerreL}\left[\frac{1}{2},x\right]$

▪ PS#3 Problem 5

Ok, let's try problem 5

In[15]:= **ans5 = DSolve[4 x^2 y''[x] + 4 x y'[x] + (4 x^2 - 1) y[x] == 0, y, x]**

Out[15]= $\left\{\left\{y\to\text{Function}\left[\{x\},\frac{e^{-ix}C[1]}{\sqrt{x}}-\frac{i\,e^{ix}C[2]}{2\sqrt{x}}\right]\right\}\right\}$

Pull out the function and convert to sines and cosines:

In[16]:= **ExpToTrig[y[x] /. ans5 [[1]]] // Simplify**

Out[16]= $\frac{(2C[1]-i\,C[2])\,\text{Cos}[x]+(-2i\,C[1]+C[2])\,\text{Sin}[x]}{2\sqrt{x}}$

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<u>Gamma</u> <u>function</u> $\Gamma(z)$ — [see Chap. 8 in Arfken; Sect 2.9 in Lea]

· In the solution to Laguerre's equation in problem 4 of PS#3, you found the series solution:

$$y(x) = a_0 \sum_{n=0}^{\infty} \frac{(-1)^n \alpha(\alpha-1)\cdots(\alpha-(n-1))}{(n!)^2} x^n$$

· How could we write the n^{th} term more generally?

· Consider $\alpha = k$, an integer:

$$\Rightarrow k(k-1)\cdots(k-(n-1)) = \frac{k(k-1)\cdots(k-(n-1))(k-n)(k-(n+1))\cdots 3\cdot 2\cdot 1}{(k-n)(k-(n+1))\cdots 3\cdot 2\cdot 1}$$

$$= \frac{k!}{(k-n)!}$$

Can we generalize? Yes, with $z! = \Gamma(z+1)$, then $\frac{\Gamma(\alpha+1)}{\Gamma(\alpha+1-n)}$ is equal to the $\alpha(\alpha-1)\cdots(\alpha-(n-1))$ part.

The Gamma function is defined as

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1}\, dt \quad \text{for } x > 0 \text{ (real)}$$

· $\Gamma(1) = \int_0^\infty e^{-t} dt = -e^{-t}\Big|_0^\infty = 1$

· We can integrate by parts to show that $\Gamma(x+1) = x\Gamma(x) = x(x-1)\Gamma(x-1)$

$$\xrightarrow{x=n \text{ integer}} \Gamma(n+1) = n!$$

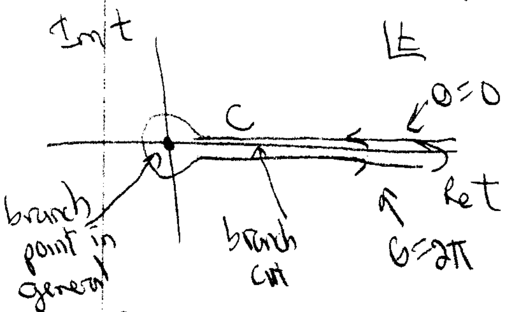
[e.g. $u = e^{-t} \Rightarrow du = -e^{-t}dt$. $dv = t^{x-1}dt \Rightarrow v = \frac{t^x}{x}$

$\Rightarrow \Gamma(x) = \cancel{e^{-t}\frac{t^x}{x}\Big|_0^\infty} + \int \frac{t^x}{x} e^{-t} dt = \frac{1}{x}\Gamma[x+1]$]

10/14/11 Note that $\displaystyle\int_{-\infty}^{\infty} e^{-u^2}\,du = 2\int_0^{\infty} e^{-u^2}\,du = 2\cdot\frac{1}{2}\int_0^{\infty} e^{-t}\, t^{-1/2}\,dt = \Gamma(1/2)\,!$

$t = u^2$, $u = t^{1/2}$, $du = \frac{1}{2}\frac{dt}{t^{1/2}}$

How do we define the integral for $\mathrm{Re}(z) > 0$? Use a contour integral.



Use this contour so that we include the top of the branch backwards and the bottom from $\mathrm{Re}\,t = 0$ to ∞, with $\theta = 2\pi$.

- The little circle around the branch point vanishes:

$$\int_{C_\varepsilon} t^{z-1} e^{-t}\,dt = \int_0^{2\pi} (\varepsilon e^{i\theta})^{z-1}\, e^{-(\varepsilon e^{i\theta})}\, i\varepsilon e^{i\theta}\,d\theta$$

$$\xrightarrow[\varepsilon\to 0]{} \varepsilon^z \int_0^{2\pi} e^{iz\theta}\, i\,d\theta$$

$$= \frac{\varepsilon^z}{z}\left(e^{2\pi i z} - 1\right) \xrightarrow[\varepsilon\to 0]{} 0 \quad \text{for } \mathrm{Re}(z) > 0$$

- On the bottom of the branch, we get an extra $e^{2\pi i z}$, so

$$\boxed{\Gamma(z) = \frac{1}{\underbrace{e^{2\pi i z}}_{\text{bottom of cut}} \underbrace{-\,1}_{\text{top of cut}}} \int_C t^{z-1} e^{-t}\,dt \qquad \boxed{\mathrm{Re}\, z > 0}}$$

When $z = n$ positive integer, define as limit. There are simple poles for $z =$ non-negative integer.

Ok, but what about $\Gamma(-1/2)$? Define by analytic continuation using

$\Gamma(z) = \Gamma(z+1)/z$ sufficiently many times. E.g. $\Gamma(-1/2) = \Gamma(+1/2)/(-1/2)$

(repeat until $\mathrm{Re}(z+1) > 0$)

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"Practical Points Concerning the Solution of the Schrödinger Equation"
- By John M. Blatt ⇒ online handout
- Numerov method (less general than Runge-Kutta but more effective for Schrödinger equation usually)

- To solve a differential equation numerically, you will usually use a "packaged" library routine, either in Mathematica or MATLAB or from a numerical library in C++, fortran, python, ...
  - But you may sometime need to implement you own solver.

- Basic plan: approximate derivatives using Taylor expansion.
  - For initial value problem, input starting value(s) and integrate (that is, solve the equation) step-by-step.
  - Works best for smooth, slowly varying function ⇒ remove rapid or non-polynomial parts if possible for greater accuracy.

- Consider solving a one-variable S-equation for a bound-state energy $E<0$:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V(x)u(x) = Eu(x) \Rightarrow \boxed{\frac{d^2u}{dx^2} = f(x)\,u(x)} \text{ with } \boxed{f(x) = \frac{2m}{\hbar^2}(V(x)-E)}$$

- Assume $V(x) \xrightarrow[x\to\infty]{} 0$ and negative somewhere (so a bound state is possible)

- Assume $u(x=0)=0$. Why?
- Want $u(x)$ to be "bounded and square-integrable" ⇒ normalizable so $\sum$ probabilities $=1$
- As a differential equation, this is linear, 2nd-order, self-adjoint (Hermitian)
  - No first derivative. Why?

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Consider the Taylor expansions about x with $\Delta x = \pm h$:

$$u(x+h) = \sum_{n=0}^{\infty} \frac{h^n}{n!} u^{(n)}(x) \qquad u(x-h) = \sum_{n=0}^{\infty} \frac{(-1)^n h^n u^{(n)}(x)}{n!}$$

We want even derivatives only $\Rightarrow$ average

$$\frac{1}{2}\left[u(x+h) + u(x-h)\right] = u + \frac{1}{2}h^2 u^{(2)} + \frac{h^4}{4!}u^{(4)} + \frac{h^6}{6!}u^{(6)}$$

no argument means "evaluate at x"

- We can eliminate $u^{(2)}(x)$ using the S-eqn: $u^{(2)}(x) = f(x)u(x)$
- We can get rid of $u^{(4)}(x)$ by differentiating the above equation and subtracting:

$$\frac{1}{2}\left[u^{(2)}(x+h) + u^{(2)}(x-h)\right] = u^{(2)} + \frac{1}{2}h^2 u^{(4)} + \frac{h^4}{4!}u^{(6)} + \dots$$

So

$$\frac{1}{2}\left[u(x+h) + u(x-h)\right] - \frac{h^2}{12}\frac{1}{2}\left[u^{(2)}(x+h) + u^{(2)}(x-h)\right]$$
$$= u + \frac{5}{12}h^2 u^{(2)} + \left(\frac{1}{6!} - \frac{1}{12\cdot 4!}\right)h^6 u^{(6)} + \dots$$

Replace $u^{(2)}$ by $f(x)\,u(x)$

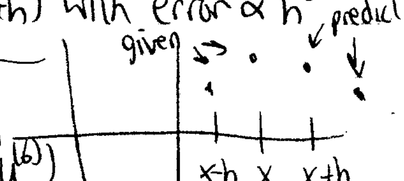
$$\Rightarrow \frac{1}{2}\left[u(x+h) + u(x-h)\right] - \frac{1}{24}h^2\left[f(x+h)u(x+h) + f(x-h)u(x-h)\right] -$$
$$= u(x) + \frac{1}{2}\frac{5}{6}h^2 f(x)u(x) - \frac{1}{480}h^6 u^{(6)} + \dots$$

Define <u>dimensionless</u> $T(x) \equiv \frac{h^2}{12}f(x) = \frac{h^2 2m}{12\hbar^2}\left[V(x) - E\right]$
and gather all the $u(x+h)$, $u(x)$, $u(x-h)$ terms: (multiply by 2)

$$\left(1 - T(x+h)\right)u(x+h) + \left(1 - T(x-h)\right)u(x-h) = \left[2 + 10T(x)\right]u(x) - \frac{h^6}{240}u^{(6)}$$

Plan: knowing $u(x-h)$ and $u(x)$, we can find $u(x+h)$ with error $\propto h^6$

$$\Rightarrow \boxed{u(x+h) = \frac{1}{1 - T(x+h)}\left[-\left(1 - T(x-h)\right)u(x-h) + \left(2 + 10T(x)\right)u(x)\right] + O\left(h^6 u^{(6)}\right)}$$



- 3-point method with high order error, stable: unlike some other rules.

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Notes:

- We need $u(0)$ and $u(h)$ [or $u(h)$, $u(2h)$] to get started: series solution!
- $T(x)$ is known but possibly only at $x = 0, h, 2h, \ldots x_{max}$
  - Wait: isn't $x_{max} = \infty$? Not on the computer. Either x_{max} is large enough that $u(x_{max}) = 0$ is a negligible distortion or one matches to a exact solution (integrating in).
- You can't just take h smaller and smaller to improve accuracy
  $\Rightarrow$ eventually round-off wins: numbers have a finite number of digits precision when stored on computers, and finer cancellations mean fewer digits precision after.

- For bound states, integrate out from the origin and in from infinity to go in the direction that $|u(x)|$ increases.
  - avoids error contributions from growing exponentially or as a power law.
  - How to find eigenvalues? (Later!)

- We can estimate errors for $V(x)$ such that $f(x)$ is slowly varying compared to the step size.
  - If $f(x)$ is positive, then $f(x) \sim +k^2$ and $u(x)$ is roughly $u(x) \sim e^{\pm\sqrt{f(x)}\,x}$
  - When $f(x)$ is negative, $u(x) \sim \sin(-\sqrt{f(x)}\,x - b)$
  - In either case
  $$u^{(6)}(x) \approx [f(x)]^3\, u(x) \qquad \left(\text{error per step is } \frac{-h^6}{240} u^{(6)}\right)$$

  so with each step, the error is

$$\Rightarrow \frac{\text{relative error}}{\text{step}} = \frac{\text{error in } u(x+h)}{u(x)} = \frac{-\frac{h^6}{240}[f(x)]^3 \cancel{u(x)}}{\cancel{u(x)}} = -\frac{2}{10}[T(x)]^3$$

So we can determine an h to use if we know how many steps is feasible and the desired tolerance. Eg. 1% accuracy and 500 steps $\Rightarrow |T(x)| \lesssim 0.01$ is an upper limit. Can adjust h to keep $T(x)$ near this limit $\Rightarrow$ Adaptive. More later!

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Fourier Series : Pass 1

- In our brief look at series solutions to differential equations, all of the equations were <u>linear</u> : only single powers of y and its derivatives.
  - Jackson, in the introduction to his text on Classical Electrodynamics, argues that linear systems are all he needs to consider.
  - More generally we have to consider scales and ensure that $y(x)$ doesn't get "unnaturally" large.
- Linearity means that given two solutions $y_1(x)$ and $y_2(x)$, the linear sum $c_1y_1 + c_2y_2$ is also a solution. E.g. for $y'' + \alpha y = 0$
  - conversely, if we have something like $y'' + \alpha y^2 = 0$, the linear combination <u>doesn't</u> work because we have cross terms.

- You recognize the physics of this property of linearity as the principle of superposition.
  - It means we can make complicated solutions by adding together simple ones
  - But also that we can decompose complicated solutions (essentially any we would encounter in a physics problem) into simple ones.

- <u>One</u> choice of simple functions for $f(x)$ in $0 \le x \le 2\pi$, [also written $x \in [0, 2\pi]$] are sines and cosines, or e^{ixn}'s

$$\Rightarrow f(x) = \underbrace{\sum_{n=0}^{\infty} (a_n \sin nx + b_n \cos nx)}_{\text{real}} = \underbrace{\sum_{n=-\infty}^{\infty} c_n e^{inx}}_{\text{complex}}$$

Core competencies:
1. finding coefficients
2. basic examples: square wave, saw tooth $\rightarrow$ behavior of series (Gibb's overshoot)
3. solving certain diff eqs (which ones, how to do it)
4.